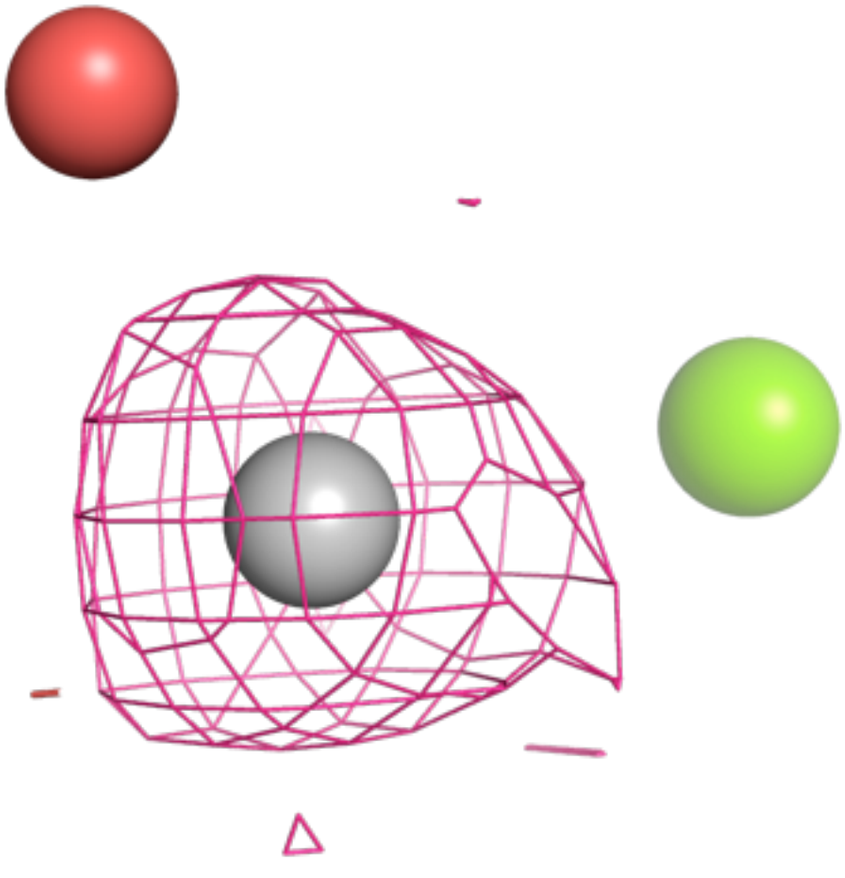
# A brief aside on anomalous refinement and maps

(with Airlie McCoy & Randy Read)

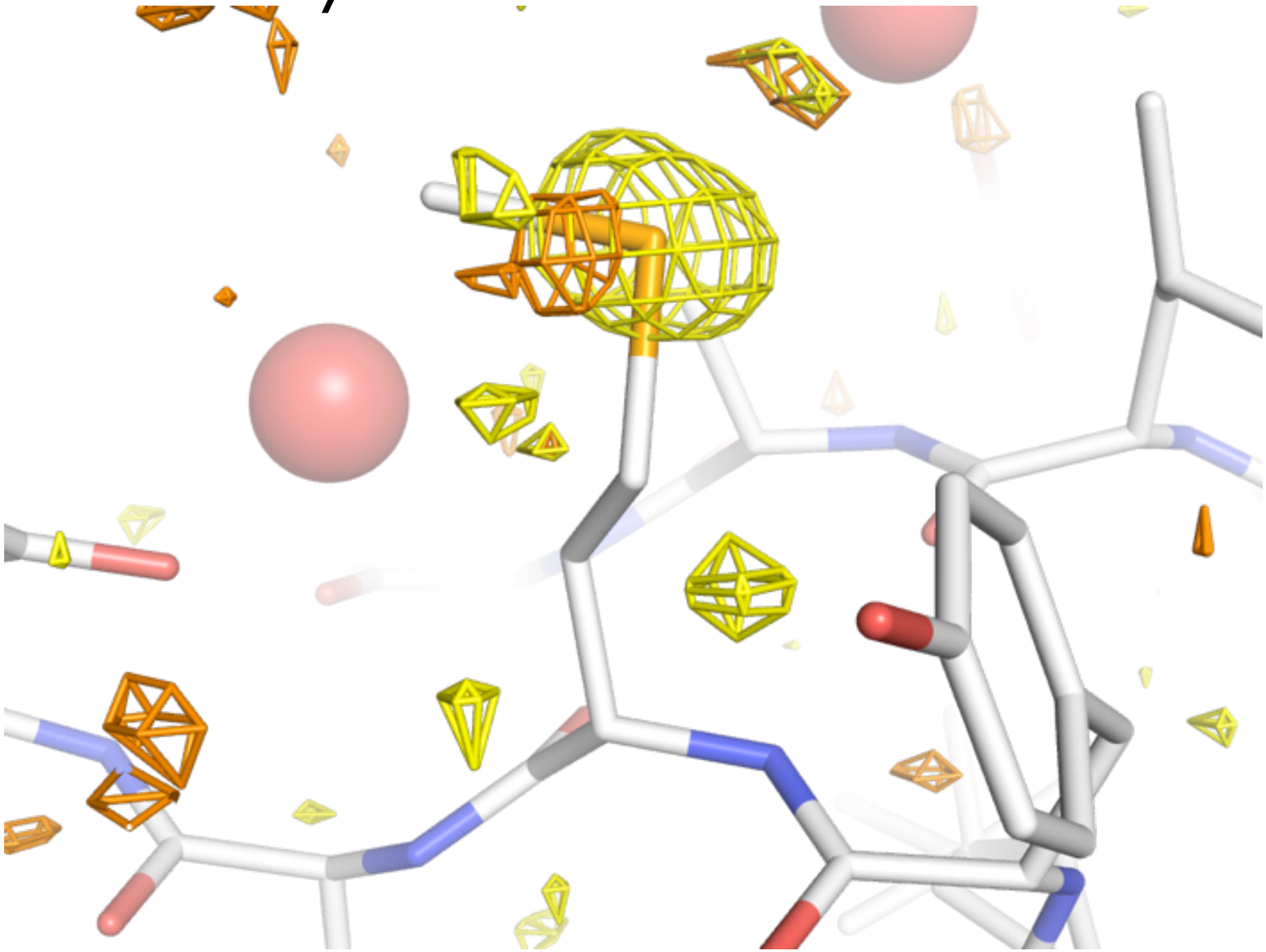


# Computing SAD LLG maps from Phenix

- Added map_type=llg (or "llgsad") in October 2012
- Using existing partially working SAD target code, with modifications
- Inputs are a PDB hierarchy and fmodel object
- Use fmodel to supply F(calc), instead of generating it fresh from the PDB hierarchy
- This will work best if anomalous groups are refined **and** contribute to F(calc)
  - but we can also guess f'/f" if wavelength is specified
- Appearance for a purely real model is similar to anomalous difference map, at least for actual anomalous groups
- Testing by calculating maps from phenix.refine after anomalous group refinement of selected heavy atoms

# LLG versus anomalous difference

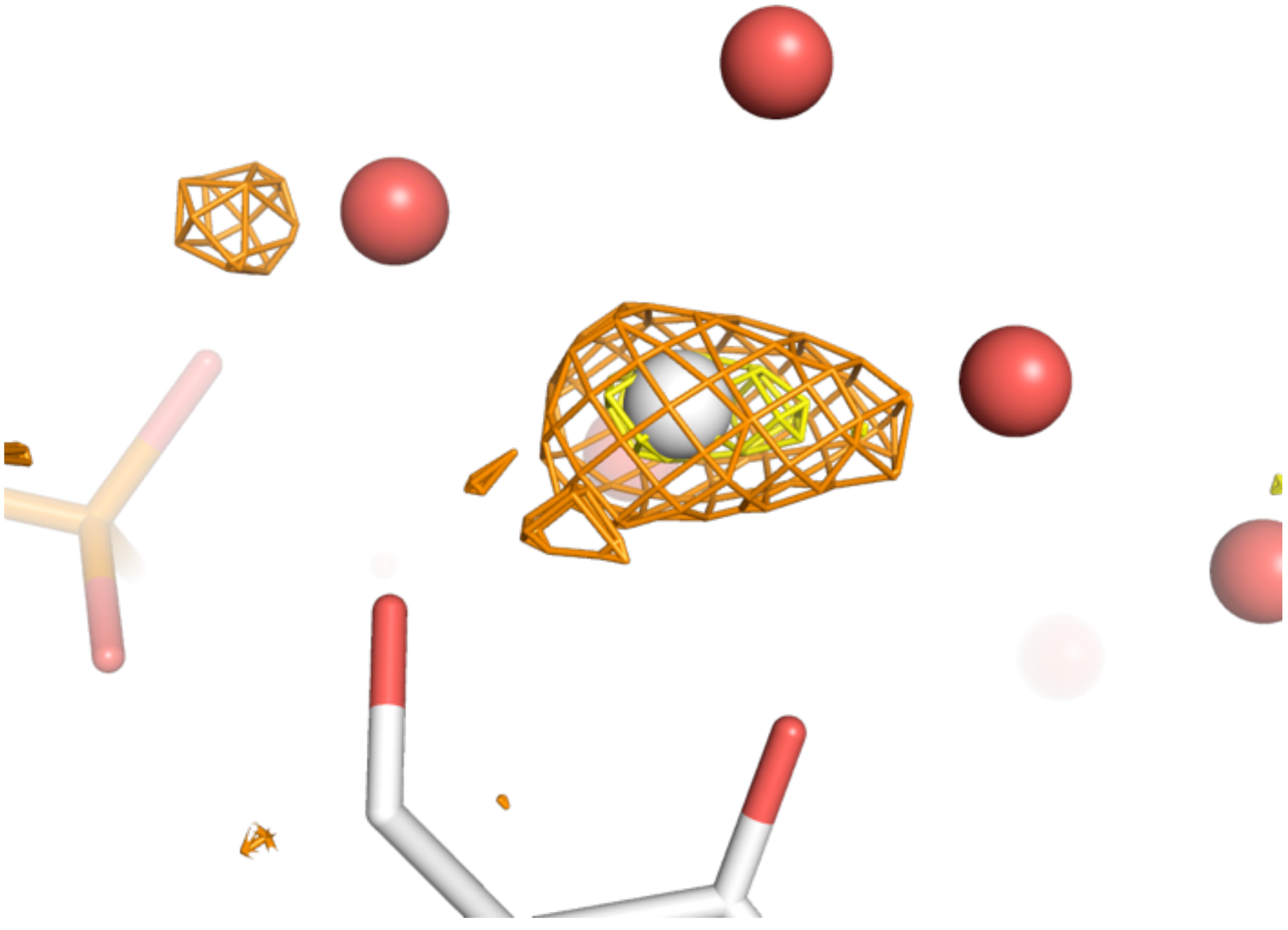
- Output from phenix.refine run of 3s6f, with f' and f" refined for Se atoms only



yellow = anomalous @ 3 sigma; orange = LLG @ 3 sigma

# LLG versus anomalous difference

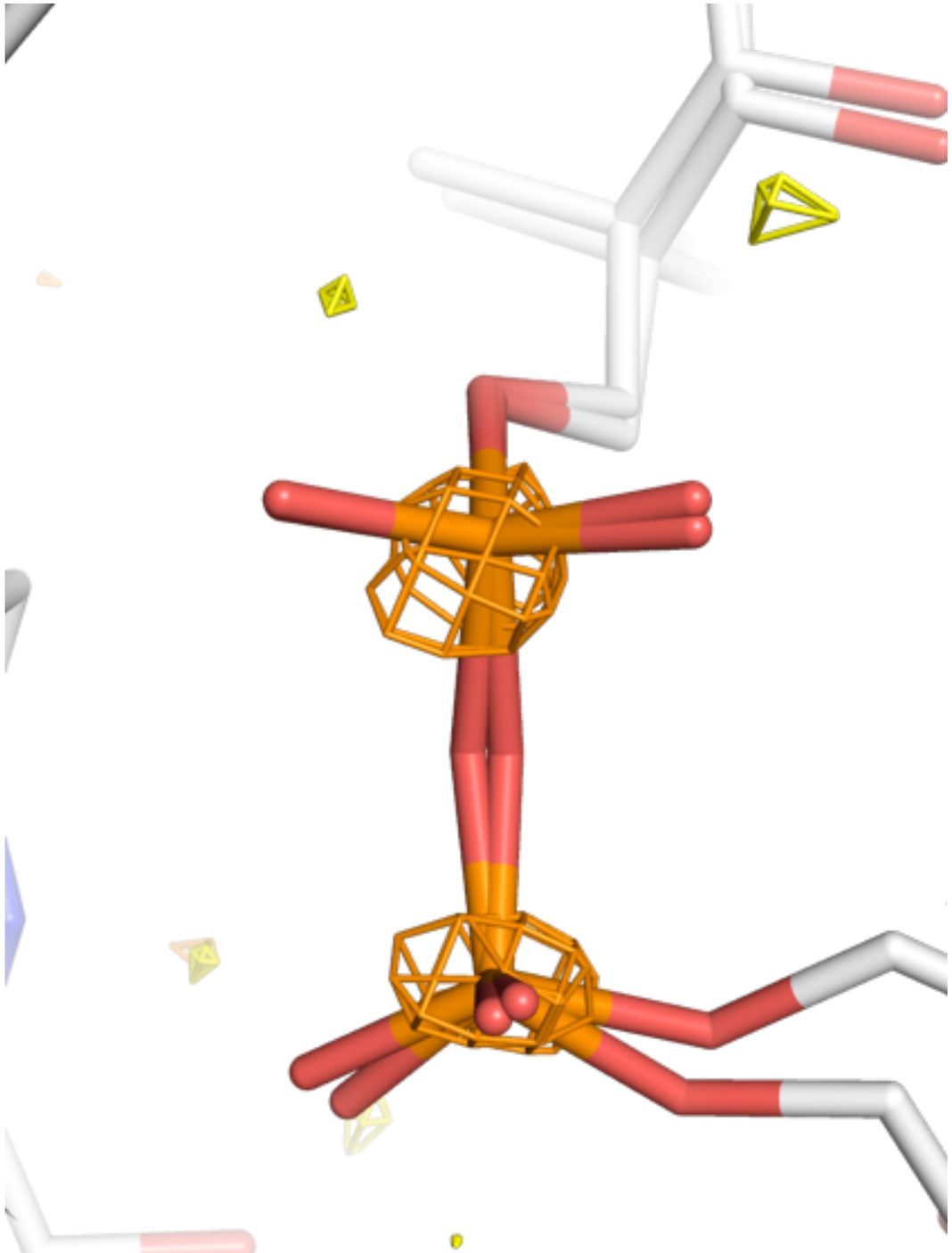
- Peak on calcium ion goes from < 5 sigma to > 10 sigma

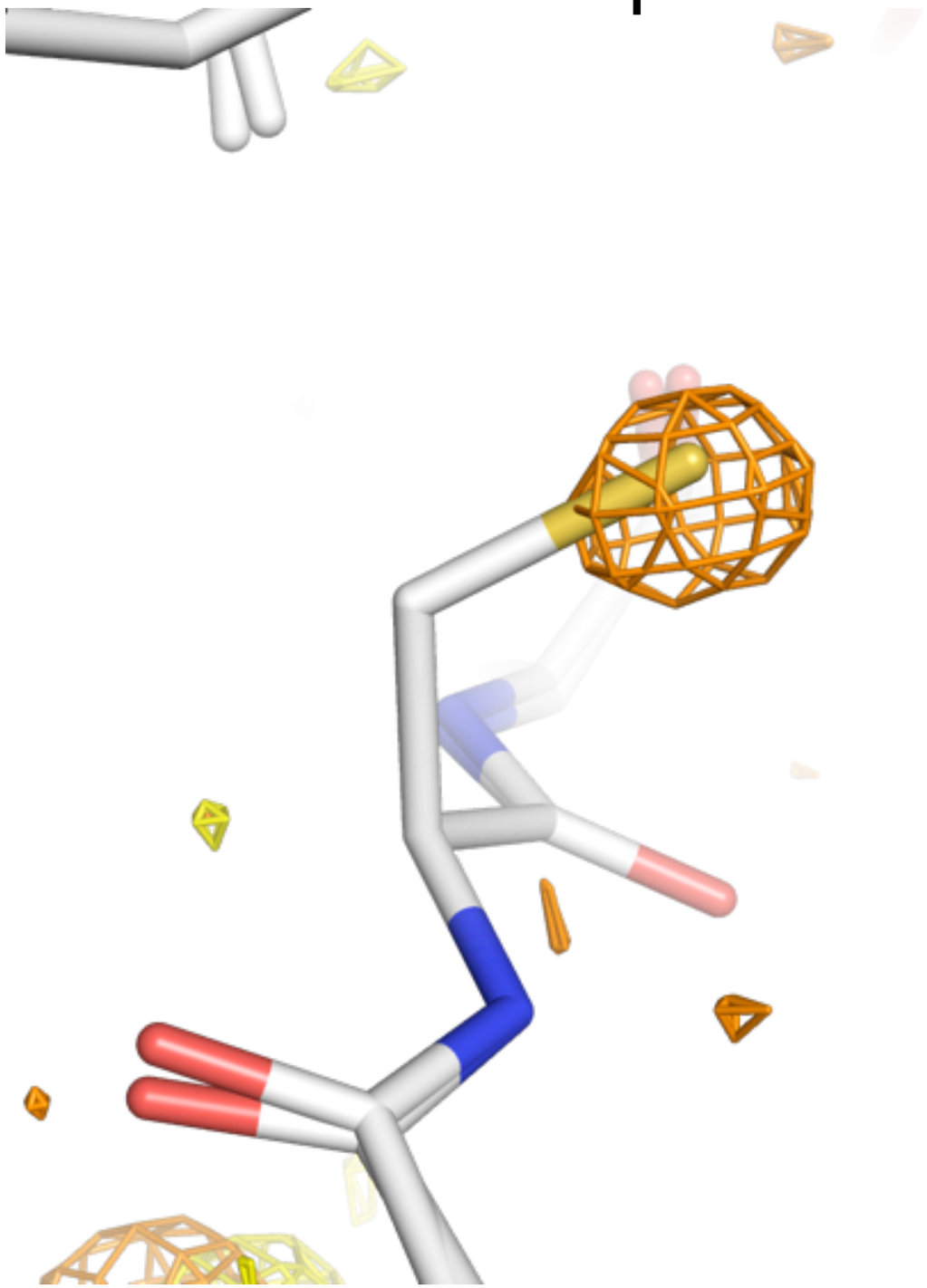


yellow = anomalous @ 3 sigma; orange = LLG @ 3 sigma

# LLG versus anomalous difference

- With anomalous scattering refined for both SE and CA, the P and S atoms in 3s6f become clear in the LLG map





# Advantages and limitations of LLG maps

- The main disadvantage of implementing the substructure completion in Python is that it's 2x slower than Phaser
- Even just calculating an LLG map by itself has a large overhead; can we get away with something simpler?
  - using an unweighted anomalous difference-difference map, 26 anomalously scattering "waters" can be picked in Ubq structure containing $CdCl_2$
  - with LLG map, 30 anomalous scatterers found
  - timings: ~25s versus ~340s (inc. anomalous refinement)
  - so Phaser's maps really are more sensitive, but at least an order of magnitude slower

# Incorporating anomalous refinement

- Theoretically all elements have anomalous scattering, but at MX wavelengths only P and higher will be detectable
- We could automatically flag any suspicious water for anomalous refinement (as well as any new ions)
- Use anomalous residual map (or LLG map) to identify
  - refined f' and f'' give us orthogonal information about identity (since f' will estimate the occupancy error in e-)
- In effect we get a crude mimic of the substructure completion in Phaser, but with chemical knowledge added
- This does in fact work - but with mixed results so far compared to Phaser